An Introduction to Statistical Mechanics and the Ising Model

- A branch of physics that deals with systems with a large number of interacting elements.
  
  Classic examples:
  - Gases
  - Fluids
  - Magnets...
  
  ⇒ Newton's Eqs.
  ⇒ Hamilton Eqs.

- A direct application of Mechanics to each of its individual parts is impossible due to the extreme size of the system - \( N \approx 10^{23} \)!

- However, if one looks at the macroscopic properties of these systems, such as P & T, they are well-behaved quantities.

  ⇒ microscopic properties must "average" out to give predictable macroscopic behavior for the whole system.
- This "averaging" property of large systems give us the ability to describe the system statistically — "statistical Mechanics".

Levels of complications

"Microcanonical Ensembles": isolated systems with no exchange of energy or particles with its environment (E is conserved here)

The energy $E$ of the system is fixed by the Hamiltonian function $H(x)$

where $x$ is a high dimensional vector that specifies the configuration of the system.

* For large systems, there might be a large number of degenerate states for a given value of $E$. 

SECTION 6.2

For the sake of simplicity, suppose that the volume $V$ of the system is its only relevant external parameter. An isolated system of this kind consists then of a given number $N$ of particles in a specified volume $V$, the constant energy of the system being known to lie in some range between $E$ and $E + \delta E$. Probability statements are then made with reference to an ensemble which consists of many such systems, all consisting of this number $N$ of particles in this volume $V$, and all with their energy lying in the range between $E$ and $E + \delta E$. The fundamental statistical postulate asserts that in an equilibrium situation the system is equally likely to be found in any one of its accessible states. Thus, if the energy of a system in state $r$ is denoted by $E_r$, the probability $P_r$ of finding the system in state $r$ is given by

$$ P_r = \begin{cases} C & \text{if } E < E_r < E + \delta E \\ 0 & \text{otherwise} \end{cases} $$

(6.1.1)

where $C$ is a constant. It can be determined by the normalization condition that $\Sigma P_r = 1$ when summed over all accessible states in the range between $E$ and $E + \delta E$.

An ensemble representing an isolated system in equilibrium consists then of states distributed in accordance with (6.1.1). It is sometimes called a "microcanonical" ensemble.

6.2 System in contact with a heat reservoir

We consider the case of a small system $A$ in thermal interaction with a heat reservoir $A'$. This is the situation already discussed in Sec. 3.6 where $A \ll A'$, i.e., where $A$ has many fewer degrees of freedom than $A'$. The system $A$ may be any relatively small macroscopic system. (For example, it may be a bottle of wine immersed in a swimming pool, the pool acting as a heat reservoir.) Sometimes it may also be a distinguishable microscopic system which can be clearly identified.* (For example, it may be an atom at some lattice site in a solid, the solid acting as a heat reservoir.) We ask the following question: Under conditions of equilibrium, what is the probability $P_r$ of finding the system $A$ in any one particular microstate $r$ of energy $E_r$?

This question is immediately answered by the same reasoning as was used in Sec. 3.3. We again assume weak interaction between $A$ and $A'$ so that their energies are additive. The energy of $A$ is, of course, not fixed. It is only the total energy of the combined system $A^{(0)} = A + A'$ which has a constant value in some range between $E^{(0)}$ and $E^{(0)} + \delta E$. The conservation of energy can then be written as

$$ E_r + E' = E^{(0)} $$

(6.2.1)

where $E'$ denotes the energy of the reservoir $A'$. When $A$ has an energy $E_r$,

* The qualifying remark is introduced because it may not always be possible to label

the reservoir $A'$ must then have an energy near $E' = E^{(0)} - E_r$. Hence, if $E'$ is in the one definite state $r$, the number of states accessible to the combined system $A^{(0)}$ is just the number of states $\Omega'(E^{(0)} - E_r)$ accessible to $A'$ when its energy lies in a range $\delta E$ near the value $E' = E^{(0)} - E_r$. But, according to the fundamental statistical postulate, the probability of occurrence in the ensemble of a situation where $A$ is in state $r$ is simply proportional to the number of states accessible to $A^{(0)}$ under these conditions. Hence

$$ P_r = C' \Omega'(E^{(0)} - E_r) $$

(6.2.2)

where $C'$ is a constant of proportionality independent of $r$. As usual, it can be determined from the normalization condition for probabilities, i.e.,

$$ \sum_r P_r = 1 $$

(6.2.3)

where the sum extends over all possible states of $A$ irrespective of energy.

Up to now, our discussion has been completely general. Let us now make use of the fact that $A$ is a very much smaller system than $A'$. Then $E_r \ll E^{(0)}$ and (6.2.2) can be approximated by expanding the slowly varying logarithm of $\Omega'(E')$ about the value $E' = E^{(0)}$. Thus

$$ \ln \Omega'(E^{(0)} - E_r) = \ln \Omega'(E^{(0)}) - \frac{\partial \ln \Omega'}{\partial E'} E_r + \cdots $$

(6.2.4)

Since $A'$ acts as a heat reservoir, $E_r \ll E^{(0)}$ and higher order terms in the expansion can be neglected. The derivative

$$ \frac{\partial \ln \Omega'}{\partial E'} = \beta $$

(6.2.5)

is evaluated at the fixed energy $E' = E^{(0)}$ and is thus a constant independent of the energy $E_r$ of $A$. By (3.3.10) it is just the constant temperature parameter $\beta = (kT)^{-1}$ characterizing the heat reservoir $A'$. (Physically, this means that the reservoir $A'$ is so large compared to $A$ that its temperature remains unaffected by whatever small amount of energy it gives to $A$.) Hence (6.2.4) becomes

$$ \ln \Omega'(E^{(0)} - E_r) = \ln \Omega'(E^{(0)}) - \beta E_r $$

or

$$ \Omega'(E^{(0)} - E_r) = \Omega'(E^{(0)}) e^{-\beta E_r} $$

(6.2.6)

Since $\Omega'(E^{(0)})$ is just a constant independent of $r$, (6.2.2) becomes then simply

$$ P_r = C e^{-\beta E_r} $$

(6.2.7)

where $C$ is some constant of proportionality independent of $r$. Using the normalization condition (6.2.3), $C$ is determined by the relation

$$ C^{-1} = \int P_r $$
"Canoical ensembles": systems are in thermal contact with a heat reservoir.

- heat reservoir is assumed to be big, so that $T_{	ext{reservoir}}$ can be considered fixed.

But, energy $E$ can be exchanged between the reservoir and the system.

- At a given temperature $T$, the system typically has access to a large # of allowed states!

Statistical Description of States

1) Let define

$$R(x \to x') \; dt$$

to be the probability that the system starting in state $x$ and ending up in state $x'$ after $dt$.

$R(x \to x')$ is called the transition rate.
\( R(x \rightarrow x') \) is usually assumed to be time independent.

2. Now, we can also define a set of weights \( W_x(t) \) that gives the probability in finding the system at state \( x \) at time \( t \).

3. Then, the time evolution of the system can be described by the "master equation":

\[
\frac{dW_x}{dt} = \sum_{x'} [W_x(t) R(x' \rightarrow x) - W_{x'}(t) R(x \rightarrow x')]
\]

- This is just a statement on the conservation of probability.

Since \( W_x(t) \) is a probability, it must also satisfy:

\[
\sum_x W_x(t) = 1, \text{ for all time.}
\]
These two equations formally define $W_x(t)$!

With $W_x(t)$ known, then all macroscopic properties can be estimated.

For example, $E(x)$ is the energy for a given state, then

$$
\langle E \rangle = \sum_x E(x) W_x(t)
$$

gives the expectation of the energy for the system.

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**Equilibrium**

Consider the situation when the rates of going into and out of $x$ exactly cancel,

then $\frac{dW_x(t)}{dt} = 0$ or $W_x(t)$ is constant in time.

- We would call the system to be in equilibrium.
Since the master equation is of 1st order and $W_x(t) \in [0, 1]$ (probability), all systems governed by this equation must approach equilibrium at large $t$.

For systems in equilibrium, $R(x \rightarrow x')$ must take on specific values!

For systems in equilibrium, we know how the equilibrium occupation probability

$$p(x) = \lim_{t \rightarrow \infty} W_x(t)$$

should behave. (Gibb 1902, Boltzmann)

In Boltzmann's constant

$$p(x) = \frac{1}{Z} e^{-\beta E(x)/kT}$$

where

$$Z = \sum_x e^{-\beta E(x)/kT} = \sum_x e^{-\beta E(x)}$$

- $Z$ is also the normalization factor.

- $p(x)$ is called the Boltzmann's distribution.
So, in terms of \( p(x) \), macroscopic averages are,

\[
\langle Q \rangle = \sum_x p(x) Q(x) = \frac{1}{Z} \sum_x Q(x) e^{-\beta E(x)}
\]

In particular, the expectation value of the energy \( \langle E \rangle \) (the internal energy of the system) is

\[
U = \frac{1}{2} \sum_x E(x) e^{-\beta E(x)}
\]

**Note**: This can also be written in terms of \( Z \),

\[
U = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta}
\]

**Check**:

\[
\frac{\partial Z}{\partial \beta} = \frac{2}{e^\beta} \left( \sum_x e^{-\beta E(x)} \right) = Z \left( -\langle E(x) e^{-\beta E(x)} \rangle \right)
\]

\[
-\frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{1}{Z} \sum_x E(x) e^{-\beta E(x)}
\]
And, specific heat is,

\[ dT = -\frac{1}{k \beta} \, d\beta \]

\[ u = -\frac{\partial \log z}{\partial \beta} \]

\[ C = \frac{\partial U}{\partial T} = -k \beta^2 \frac{\partial U}{\partial \beta} = k \beta^2 \frac{\partial^2 \log z}{\partial \beta^2} \]

Recall \( \beta = \frac{1}{kT} \)

Then, from thermodynamic relations, we have

\[ C = T \frac{\partial S}{\partial T} = -\beta \frac{\partial S}{\partial \beta} \]

So,

\[ S = \int -\frac{C}{\beta} \, d\beta \]

\[ = -\int k \beta \frac{\partial^2 \log z}{\partial \beta^2} \, d\beta \]

\[ u = k \beta \]

\[ du = \frac{\partial^2 \log z}{\partial \beta^2} \, d\beta \]

\[ dv = \frac{\partial \log z}{\partial \beta} \]

\[ d\mu = k \, d\beta \]

\[ v = \frac{\partial \log z}{\partial \beta} \]

\[ = -k \beta \frac{\partial \log z}{\partial \beta} + \int \frac{\partial \log z}{\partial \beta} \, k \, d\beta \]

\[ S = -k \beta \frac{\partial \log z}{\partial \beta} + k \log z \]
Then, the free energy is given by

\[ F = U - TS = - \frac{\partial \log Z}{\partial \beta} - \frac{1}{k_B} \left( -k_B \frac{\partial \log Z}{\partial \beta} + k_B \beta Z \right) \]

\[ = -kT \log Z \]

Then, with \( \Gamma \), we can calculate all the "conjugate" forces to the system:

\[ P = -\frac{\partial F}{\partial V} \]

\[ M = \frac{\partial F}{\partial \beta} \]

\( (P, V) \quad (M, \beta) \)

\( Z \) (the partition function) is an important quantity in statistical physics.

In numerical simulations, it is important to be able to calculate \( Z \) accurately!

- All macroscopic thermodynamic quantities can be derived by taking the appropriate derivatives of \( Z \) with respect to \( P, V, \beta \), etc.
Calculating \( C \) more directly:

Consider the variance of \( E \):

\[
\langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - 2\langle E \rangle \cdot \langle E \rangle + \langle E \rangle^2
\]

\[
= \langle E^2 \rangle - 2\langle E \rangle^2 + \langle E \rangle^2
\]

\[
= \langle E^2 \rangle - \langle E \rangle^2
\]

Now, \( \langle E \rangle = \frac{1}{2} \int \frac{E}{2} \ e^{-\beta E(x)} \ dx \)

\[
= \frac{1}{2} \int \frac{2}{\beta^2} \ dx
\]

\[
= \frac{1}{2} \left( \frac{2}{\beta^2} \right)^2
\]

Note:

\[
\frac{\partial}{\partial \beta} \left( \frac{\partial^2 \rho}{\partial \beta^2} \right) = \frac{2}{\beta^2} \left( \frac{1}{2} \frac{\partial}{\partial \beta} \right)
\]

\[
= \frac{1}{2} \frac{\partial^2 \rho}{\partial \beta^2} - \frac{1}{2} \frac{\partial}{\partial \beta} \frac{\partial}{\partial \beta}
\]

\[
\frac{C}{k\beta^2} = \langle E^2 \rangle - \langle E \rangle^2
\]
The Ising Model

- A simple model for a magnet.

Model

\[
\begin{array}{cccc}
S_i & S_j & S_k & S_l \\
\end{array}
\]

- Macroscopic magnetism is resulted from a collection of magnetic dipoles or atomic spins \( S_0 \).

- The spins are assumed to be in a fixed lattice (3D physical, 2D simplified system chain).

Note: 1D & 2D can be solved analytically (Onsager, 1944). 3D is still unresolved analytically.
This system is characterized by the Hamiltonian

\[ H = -2 \vec{z} \cdot \vec{s} - \frac{1}{2} \gamma S^z \]

The system is in a pseudo-magnetic state as the spin phase transition is paramagnetic.

A model provides a picture of how
- interactions are of the nearest neighbor type.
- Continuous spin models such as
  - Heisenberg 2D
  - Other types exist such as
    - can be up (+1) or down (-1)

\[ \text{Eq.}(12) \]
Then, the partition function is given by

$$Z = \sum_{\{\mathbf{S}_i\}} e^{-\beta H}$$

up

summing all possible combinations of \(\{\mathbf{S}_i\}\)

with a given energy \(E(=H)\).

- \(\langle M \rangle = \langle \sum_{i} \mathbf{S}_i \rangle \) over ensemble

mean magnetization

- \(\langle m \rangle = \frac{\langle M \rangle}{N}\)

mean magnetization per spin
Counting Bonds on Ising Grid

\[ H = - \sum_{\langle ij \rangle} S_i S_j \]  
sum over all bonds

with periodic boundary

For \( N \times N \) grid, \( H = -2N^2 \) for all up or down arrangement.

\(- N = 3 : \)

- 3x3 vertical bonds
- 2x3 horizontal bonds
- 2x3x3 total bonds

\[ H = -18 \]

- With one spin flip at middle

\[ E_x' = E_x + 2J \sum_{i,j} \sum_{x} S_i^x S_j^x \]

\[ = -18 + 8 = -10 \]

6 actual count = 10
0
4

\[ E_x' = -10 \]